Band Gaps for Atoms in Light based Waveguides

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The energy spectrum for a system of atoms in a periodic potential can exhibit a gap in the band structure. We describe a system in which a laser is used to produce a mechanical potential for the atoms, and a standing wave light field is used to shift the atomic levels using the Autler-Townes effect, which produces a periodic potential. The band structure for atoms guided by a hollow optical fiber waveguide is calculated in three dimensions with quantised external motion. The size of the band gap is controlled by the light guided by the fiber. This variable band structure may allow the construction of devices which can cool atoms. The major limitation on this device would be the spontaneous emission losses.

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I. INTRODUCTION

Band gaps in the energy spectrum of electrons cause many interesting effects in solid state physics, and there may be interesting devices that can be constructed using similar effects in atom optics. This paper describes a system that can produce gaps in the energy spectrum, and calculates its three dimensional energy spectrum.

Standing wave laser beams produce a periodic potential which has been used extensively in atom optics, particularly in cooling experiments utilising the Sisyphus effect [1–3]. Atoms in a periodic potential have an energy spectrum consisting of bands [4]. Experiments and theoretical calculations concerning these systems have been conducted in one and two dimensions. Three dimensional optical lattices have been investigated experimentally [5], but the quantised atomic motion has not been calculated except in the limit of very deep potential wells [6]. We present a numerical calculation of the energy spectrum of atoms in a three dimensional waveguide. This paper shows that the band structure of these atoms can be manipulated to produce an energy gap between the lowest bands.

We consider atoms that are strongly confined in two dimensions and relatively free to travel in a single direction. Hollow optical fibers have been suggested as a practicable method of guiding atoms coherently [7–9]. A laser is guided along the fiber and the evanescent field in the interior of the waveguide interacts with the dipole moment of the atoms to form a potential barrier. A naive method for producing a periodic potential would be to guide a standing wave along the fiber, but this allows atoms to absorb a photon from one beam and emit a photon into the counterpropagating beam. The associated recoil is larger than the kinetic energy of the atoms in the lowest band, so it would destroy any interesting effects. To avoid this, a second laser beam is introduced into the fiber to shift the atomic energy levels by the Autler-Townes effect. This produces a periodic potential without momentum diffusion. We present a detailed calculation of the band structure of atoms guided by a hollow optical fiber, although our model may be applied to some free space laser configurations.

In section II we derive the potential seen by the atoms under the influence of the two laser fields. In section III we present a short revision of the band structure expected for an atom in a one dimensional sinusoidal potential. Section IV describes the calculation of the atomic energy spectrum in the three dimensional fiber. The effects of spontaneous emission are estimated later and are found to be the critical factor which will limit experimental realisation of such devices. Section V describes some possible generalizations of this work to other laser configurations, and sectionVI describes some applications of controllable band structure for the atoms in a hollow optical fiber. In particular, a technique is described which can cool atoms.

II. THE POTENTIAL IN A HOLLOW OPTICAL FIBER

When the external motion of an atom is treated classically, an atom in a highly detuned light field will experience an effective potential that is proportional to the intensity of the field and inversely proportional to the detuning of the field. It follows that a standing wave light field will produce a periodic potential. When the atoms are extremely cold, there is a second effect which dominates the motion. The standing wave allows atoms to absorb and emit photons in either direction, which means that the atoms will diffuse in momentum as well as experiencing an effective potential. To avoid this momentum diffusion, we introduce a periodicity in the detuning rather than in the intensity of the field. We add a second laser beam in a standing wave, which shifts one of the atomic levels by the Autler-Townes effect [10,11].

Our atom is a three level atom with levels $|a\rangle$, $|b\rangle$ and $|c\rangle$ as shown in Fig. 1. There is a laser beam highly blue detuned from the $|a\rangle \leftrightarrow |b\rangle$ transition with detuning Δ and frequency ω_l as shown, and a second laser beam blue detuned from the $|b\rangle \leftrightarrow |c\rangle$ transition with a frequency

ω_{l2} and a much smaller detuning δ. The second laser beam, which is closer to resonance, mixes levels $|b\rangle$ and $|c\rangle$ into the dressed states $|1\rangle$ and $|2\rangle$, as shown in Fig. 2. When the Rabi frequency of the second laser is much larger than its detuning, these states are approximately given by [12]

$$|1\rangle = \frac{1}{\sqrt{2}}\left(|b\rangle + |c\rangle\right) \tag{1a}$$

$$|2\rangle = \frac{1}{\sqrt{2}}\left(|b\rangle - |c\rangle\right). \tag{1b}$$

The first laser is now detuned by an amount δ_j from the dressed state $|j\rangle$, as shown in Fig. 2. These detunings are given by

$$\delta_1 = \Delta - \frac{\sqrt{\Omega(\mathbf{r})^2 + \delta^2} - \delta}{2} \tag{2a}$$

$$\delta_2 = \Delta + \frac{\sqrt{\Omega(\mathbf{r})^2 + \delta^2} + \delta}{2}, \tag{2b}$$

where $\Omega(\mathbf{r})$ is the resonant Rabi frequency of the second laser interaction.

The second laser is chosen so that it has a frequency which is so far detuned from any transition from the ground state $|a\rangle$ that it doesn't interact with it. The frequency of the confining laser is chosen so that it is too far off resonance to interact with the $|c\rangle \leftrightarrow |b\rangle$ transition. The interaction between the second laser and the atom is much stronger than that of the first laser because it is stronger and much closer to resonance, so we use the dressed state picture and treat the interaction of the first laser semiclassically as a perturbative, electric dipole interaction. This means that the coherent motion of a single atom can be found from the Hamiltonian:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2M} + \hbar(\omega_l - \delta_1)|1\rangle\langle 1| + \hbar(\omega_l - \delta_2)|2\rangle\langle 2| + dE(\hat{\mathbf{r}}, t)\left(|b\rangle\langle a| + h.c.\right) \tag{3}$$

where $\hat{\mathbf{p}}$ is the momentum operator, M is the mass of the atom, ω_l is the frequency of the first laser, d is the dipole moment of the $|a\rangle \leftrightarrow |b\rangle$ transition, and $E(\hat{\mathbf{r}}, t)$ is the electric field due to the first laser.

If $E(\hat{\mathbf{r}}, t)$ represents a beam propagating in the +z direction then it will be of the form

$$E(\hat{\mathbf{r}}, t) = \frac{C(\hat{x}, \hat{y})}{2}\left(e^{-i(\omega_l t - k\hat{z})} + e^{i(\omega_l t - k\hat{z})}\right) \tag{4}$$

where $C(\hat{x}, \hat{y})$ is the transverse profile of the electric field. We expand $|b\rangle$ and $|c\rangle$ into the dressed states $|1\rangle$ and $|2\rangle$ and enter an interaction picture with $\hat{H}_o = \hbar(\omega_l|1\rangle\langle 1| + (\omega_l - \delta_2)|2\rangle\langle 2|)$. We then ignore terms like $|2\rangle\langle a|e^{-i\delta_2 t}$ and $|a\rangle\langle 1|e^{-i2\omega_l t}$ because δ_2 and ω_l are assumed to be large enough that these terms rotate too fast to effect the long term dynamics of the atoms. After this rotating wave approximation, the interaction Hamiltonian becomes:

$$\hat{H}_I = \frac{\hat{\mathbf{p}}^2}{2M} - \hbar\delta_1|1\rangle\langle 1| + \frac{dC}{2\sqrt{2}}\left(|1\rangle\langle a|\langle a|e^{ik\hat{z}} + h.c.\right). \tag{5}$$

In momentum space this interaction couples the states $|a\rangle|q\rangle$ and $|1\rangle|q+k\rangle$, where $|q\rangle$ is the z-momentum eigenstate with momentum $\hbar q$. The Schrödinger equation for the atom is therefore reduced to two coupled partial differential equations. We then adiabatically eliminate the excited state [13]. This is valid provided the detuning energy $\hbar\Delta$ is sufficiently large compared to the transverse, recoil, and doppler kinetic energies; provided we are only interested in time scales longer than the inverse of these detunings, and provided the population in level $|1\rangle$ is sufficiently small. The wavefunction of the $|1\rangle|q+k\rangle$ state can then be written in terms of the wavefunction of the $|a\rangle|q\rangle$ state. This gives the equation of motion for the ground state wavefunction of the atom $\Psi_a(x, y)$:

$$i\hbar\partial_t\Psi_a = -\frac{\hbar^2}{2M}\left(\partial_x^2 + \partial_y^2\right)\Psi_a + \frac{d^2C^2}{8\hbar\delta_1}\Psi_a. \tag{6}$$

The last term is an effective potential. The adiabatic elimination requires that the excited state population be very small which is equivalent to ensuring that $(\hbar d^2/4)(C/\delta_1)^2 \ll 1$. Reducing the population of the excited state is also equivalent to reducing the spontaneous emission rate of the atom. The potential barrier is proportional to C^2/δ_1, and can therefore be made large independently by making the laser stronger and detuning further.

Substituting Eq.(2a) for δ_1 into Eq.(6), we see that the effective potential $V(\mathbf{r})$ experienced by the atom is given by

$$V(\hat{\mathbf{r}}) = \frac{d^2C(\hat{x}, \hat{y})^2}{8\hbar\left(\Delta - \frac{1}{2}(\sqrt{\Omega(\hat{\mathbf{r}})^2 + \delta^2} - \delta)\right)} \tag{7}$$

The hollow optical fiber becomes an atomic waveguide when it is guiding a travelling wave laser beam which is blue detuned from a single transition in the atoms [7,8]. In this case both fields only depend on the longitudinal (z) and radial (r) coordinates.

The energy spectrum of atoms in the fiber can be calculated numerically when the potential can be separated: $V(z, r, \phi) = V^z(z)V^r(r)$. We will assume this to be true from this point. This is an approximation which becomes increasingly valid as the hole in the fiber becomes smaller, as we will now show. As previously noted, the second laser beam must have a frequency which is significantly different to the confining laser beam so that it does not interact with the confining transition. In particular, the second laser can have a much longer wavelength, and it will therefore have a different spatial mode in the fiber. When the diameter of the hole in the fiber becomes less than the wavelength of the second laser beam, the beam will have a much lower radial dependence. When the radial dependence of the intensity of the second laser beam

can be ignored then the potential given in Eq.(7) is separable. In reality, the second beam will reduce in intensity towards the center of the fiber. This will cause the confining laser to have a larger detuning from the atoms in the center, so the effect of including this in the model would be to cause the atoms to be located in a deeper potential well with a lower spontaneous emission rate. These effects should improve the practicality of an experiment, and are therefore not important for a proof of principle calculation.

III. ATOMIC ENERGY SPECTRUM IN ONE DIMENSION

If an atom is considered to be a plane wave travelling in a single dimension, and there is a sinusoidal potential in that dimension, then the solution to the Schrödinger equation is well known [14,15]. Bloch's theorem states that for a Hamiltonian of the form

$$\hat{H} = -\frac{\hat{p}^2}{2M} + V(\hat{x}), \tag{8}$$

the eigenstates $\Psi_k(x)$ of an atom in any potential with period τ in the direction x must be of the form:

$$\Psi_k(x) = e^{ikx} \sum_{n=-\infty}^{\infty} A_n e^{-i2\pi nx/\tau} \tag{9}$$

where A_n are coefficients.

This leads to the eigenvalue equation:

$$\sum_{n=-\infty}^{\infty} [-k_n^2 + \frac{2M}{\hbar^2}(E_k - V)] A_n e^{-i2\pi nx/\tau} = 0, \tag{10}$$

$$\text{where } k_n^2 = (k - 2\pi n/\tau)^2.$$

When the variation in the potential is much less than the kinetic energy of the particle, then the potential term in the above equation can be treated perturbatively, and terms with the product of V and $A_{n\neq 0}$ can be neglected. For a sinusoidal potential, it has been shown [14] that the energy spectrum is approximately $E_k = \hbar^2 k^2/2M$ except for the region $k \approx \pm\pi/\tau$, where there is a gap equal to the height of the modulation of the potential. This band gap causes interesting conductive properties in solids.

The real potential is not one dimensional. In three dimensional waveguides, variations of the potential in the transverse direction can alter or remove the gap in the band structure. The one dimensional model ignores all transverse modes. There are non-degenerate transverse modes in the three dimensional model, so their spacing must be large enough so that the gaps in the energy spectrum are not covered. From consideration of a particle in a box, where the energy spacing decreases as the size of the box increases, this will mean that the fiber will have some maximum inner radius.

IV. ATOMIC ENERGY SPECTRUM IN THREE DIMENSIONS

The energy spectrum for the three dimensional waveguide will now be calculated. The time independent Schrödinger equation in cylindrical co-ordinates (z, r, ϕ) is:

$$\left[\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}\right) + \frac{2M}{\hbar^2}\left(E - V(z,r)\right)\right]\Phi(z,r,\phi) = 0, \tag{11}$$

where Φ is the atomic eigenstate with energy E in the potential $V(z,r) = V^z(z)V^r(r)$. The absence of a ϕ component of the potential allows the eigenstate to be separated: $\Phi(z,r,\phi) = \Psi(z,r)\Theta(\phi)$. Eq.(11) can then be separated into functionally independent sides which then give a simple analytic solution for $\Theta(\phi)$, and an eigenvalue equation for $\Psi(z,r)$:

$$\Theta(\phi) = e^{im\phi} \tag{12}$$

where m is an integer, and

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} - \frac{\partial^2}{\partial z^2} + \frac{2M(V-E)}{\hbar^2} + \frac{m^2}{r^2}\right]\Psi = 0. \tag{13}$$

This shows that the rotational modes induce an effective radial potential. This equation cannot be further separated, as the longitudinal "ripple" in the potential couples the radial and longitudinal motion. With a non-zero potential this equation must be solved numerically. The details of this calculation are given in appendix A.

The light induced potential on the two level atoms is proportional to the intensity of the electric field. For fibers with hole radii larger than a few wavelengths, the evanescent field decays exponentially from the walls. For fibers with sub-micron hole radii, the radial dependance of the electric field must be calculated numerically for each fiber. This was done using the techniques described in references [7] and [16].

Gravity was neglected in this model, as the small hole size implies that the effect will be a weak perturbation. An estimate of the size of this perturbation is $\Delta E = Mg\Delta h$ which for Helium confined to a 0.5μm region is about three orders of magnitude smaller than the recoil energy. The effect of the Casimir-Polder force is approximated by reducing the potential at the walls of the fiber. Reference [7] gives an estimate that this force halves the height of the potential barrier seen by the atoms as they try to reach the surface of the glass. This change in the potential will increase the required laser power, but this system already assumes that the atoms are well confined, so the results of this model will not depend on an accurate description of this force.

The parameters chosen for the calculation were based on a commonly used transition in metastable Helium ($2^3S - 2^3P$) with a wavelength of 1083nm, but the qualitative results will not depend strongly on the chosen transition, and it is quite possible that experiments would be based on a different transition or a different atom. The calculations were made using a fiber with a step profile refractive index with core and cladding refractive indices of 1.5 and 1.497 respectively. The radial width of the core was 3μm.

The Helium atoms in the fiber exhibit a band gap in their energy spectrum for sufficiently small hole radii. Fig. 3 shows the energy spectrum of atoms in a typical fiber with increasing hole radius. The solid lines show the allowable energies, and the disallowed energies are indicated by a shading on the energy axis. Each line designates a band, and the disallowed energies are the band gaps. For small hole radii, it is clear that there is a band gap between the lowest bands, which becomes smaller as the hole becomes larger and the intensity of the light in the fiber gets lower. The spacing of the tranverse modes is clearly smaller than the spacing of the rotational modes, as the first excited rotational mode $m = 1$ (dashed line) is higher than the excited transverse modes. Only the first few $m = 0$ modes have been shown, as there is only a significant band gap between the lower bands.

As the size of the hole in the fiber approaches the de Broglie wavelength ($\lambda_{dB} = h/p$) of the recoil cooled atoms, the transverse energy spacing reduces such that the gap in the energy spectrum is closed. Small perturbative coupling between the transverse modes would allow atoms to be excited from the lowest band if such transitions were energetically allowed. These couplings may arise from interatomic collisions, gravitational, electric or magnetic fields or by imperfections in the fiber or beam. This means that the atoms will only be confined to a single band if there is a band gap. This will only occur when the hole is smaller than some maximum hole radius which is about 1.5μm for this particular system. Fig. 3(c) shows the energy spectrum for a radius which is 1.0μm, and the higher rotational mode has nearly covered the band gap. Fibers have already been manufactured with hole diameters as small as 2.0μm.

While the atoms are in the fiber, the modulation depth can be varied by altering the relative intensties of the two counterpropagating laser beams which cause the level shift. This controls the shape of the energy bands and the size of the band gap. Fig. 4 shows the effect of decreasing the modulation depth. As the modulation decreases, the lowest band becomes lower and has more range while the energy gap becomes smaller.

The large modulations cause spontaneous emission to be increased due to the reduction in detuning of the first laser beam, and in fact spontaneous emission is the key difficulty with this device. Spontaneous emission losses depend sensitively on the energy of the atoms, the size and refractive index profile of the fiber, the available power in the confining laser and its detuning from the dressed state transition. The interesting atoms are those with an energy that places them in the lowest band. Classically these atoms cannot enter the field further than the point where the potential equals their total energy. This means that an over-estimate of the spontaneous emission rate can be found by considering the spontaneous emission rate of an atom sitting at that point of maximum classical potential with the minimum detuning of the confining laser.

For a hole diameter of 1.5μm, the spontaneous emission rate is of the order of 1 Hz, given 3 W of guided laser power. This is much larger than that which might be achieved in free space, as there is quite a large field at the center of the fiber which is causing the atoms to become excited even when they are at the minimum of the potential. As may be the case for systems discussed in the next section, if there was no electric field at the center, the spontaneous emission rate would be as low as 0.01 Hz. The recoil cooled atoms would take several seconds to pass through a few centimeters of fiber, so attaining this limit for the spontaneous emission rate may be enough to produce a practical device.

V. ALTERNATIVE LASER SCHEMES

The purpose of the confining potential is to confine the atoms to a sufficently small area so that the splitting of the transverse modes is larger than the size of the lower bands. This allows a band gap to form due to the periodic potential, and the gap is not filled by higher transverse modes. It should therefore be possible to generalize this work to other designs for the physical layout of the confining laser fields.

An alternate design to the hollow optical fiber experiment is a variation on the traditional optical molasses apparatus. A standing wave in each of the two transverse directions produces a square sided "tunnel" in the laser field down which the atom can be guided. A longitudinal laser beam can then be used to produce the periodic potential. A significant advantage of this system is that there would be zero electric field at the center of the atomic waveguide. This should allow lower spontaneous emission losses, as described in the previous section. The lack of rotational symmetry in this system produces a calculational problem, however, as the potential cannot be separated. This means that an accurate calculation of the atomic energy spectrum would be difficult to do numerically.

Other free space configurations may be used. In particular, it might be possible to produce a "donut" laser mode which has a node in the center but retains the rotational symmetry which is useful in making accurate calculations.

VI. APPLICATIONS AND DISCUSSION

The existence of a band gap in the energy spectrum for the atoms will naturally suppress the excitation of atoms beyond the upper limit of the band. This means that atoms will tend to travel along the fiber with less heating from incoherent sources. Spontaneous emission losses will dominate the loss of atoms from the system, and these cannot be removed without using arbitrarily large laser powers [13], so it is not feasible to construct arbitrarily long waveguides. The most important feature of the band structure in the fiber is that it can be altered externally by changing the second laser beam. This means that interesting behaviour can be produced by changing the band structure while atoms are in transit through the waveguide.

The lowest band gap appears when the wavelength of the atoms is that of the second laser beam. This is illustrated in Fig. 4(c), where the gap between the first two bands occurs at $k/k_o = 1$. This means that a beam of atoms which are cooled close to the recoil limit will have a large population in the lowest energy band. Since the atoms are moving at speeds of the order of 3 mm/s, an atomic beam would take several seconds to pass through a centimeter of fiber. This means that the band structures can be changed so slowly that no non-adiabatic heating effects need to be considered.

It can be seen from Fig. 4 that increasing modulation depths reduce the width of the lowest energy band at the same time as increasing the band gap. If the modulation of the second laser was slowly increased while there were atoms in that band, then the atoms would have a lower energy spread. This means that while atoms are guided through the fiber, their energy spectrum can be altered in such a way that they will be cooled. This process is not expected to be necessarily competitive with other cooling processes, but it is an example of using the dynamic nature of the band structure in this fiber. A band structure with gaps in the energy spectrum which can be controlled externally is a novel situation, and may lead to other interesting effects. Our cooling mechanism is similar to an effective three dimensional cooling system which takes atoms in very deep potential wells and adiabatically reduces the depth of the wells until they are in free space [6]. This other adiabatic cooling system may be an effective method of populating the lowest energy band.

The major limitation of this system is the spontaneous emission of the atom from the excited state. This can be made arbitrarily small by increasing the detuning and the laser power, but if the laser is detuned too much then it will interact with other levels in the atom. For atoms cooled close to the recoil limit, the spontaneous emission is limited by the maximum allowable detuning.

As spontaneous emission losses are likely to be quite high unless a very low frequency transition can be used, there is some advantage to using transitions based on metastable lower states. Detectors of these atoms rely on their large excitation energy. If these atoms spontaneously emit and do not return to the metastable state, then they will not be detected, so the atoms that did not experience the correct potential will have a reduced signal. This alleviates the problem of the high spontaneous emission rate experienced by the atoms.

There are also possible methods for reducing the spontaneous emission rather than simply eliminating the incoherent signal. An example of such a modification might be to use the potential produced by a Raman transition instead of a single photon transition [13]. When extremely high laser powers can be used to produce very low potential barriers of the order of the recoil energy of the atoms, the spontaneous emission rate is limited by the fact that the allowable detuning has a maximum value beyond which the confining laser will interact with different transitions. This may be the situation for the free space configuration described in the previous section. In this case the Raman scheme has been shown to allow reductions of the spontaneous emission rate by removing this constraint.

VII. CONCLUSIONS

This paper has shown that the energy spectrum for atoms guided through a hollow optical fiber has at least two distinct bands separated by an energy gap if the radius of the hole in the fiber is less than 1.5μm. The size of this band gap and the energy range of the lowest band may be controlled externally by altering the amount of modulation of the second laser beam.

The ability to control the size of the band gap dynamically while the atoms are in the system leads to many new possibilities. This situation does not exist in solid state physics where the band structure is fixed. For example, slowly increasing the band gap while the atoms are being guided by the fiber will result in a "squeezing" of the lowest energy band, so if the atoms were originally cool enough to have a significant population in this band then they will be further cooled. The major limitation of this system is that there would be a loss due to spontaneous emission. Further work may be useful in determining whether a similar system using lasers in free space can produce similar or perhaps better results.

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APPENDIX A: DETAILS OF BAND STRUCTURE CALCULATION

In section IV the Schrödinger equation was shown to reduce to the two dimensional equation:

$$\left[-\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}+\frac{m^2}{r^2}-\frac{\partial^2}{\partial z^2}+\frac{2M(V-E)}{\hbar^2}\right]\Psi=0. \tag{A1}$$

In the full three dimensional case, shown in Eq.(11), the longitudinal co-ordinate satisfied the conditions for Bloch's theorem. The shift to cylindrical coordinates and solution of one of the degrees of freedom has not changed that fact, so we make the substitution:

$$\Psi_k(r,z)=e^{ikz}\sum_{l=-\infty}^{\infty}A_l(r)e^{-i4\pi lz/\lambda} \tag{A2}$$

This leads to the eigenvalue equation:

$$\sum_l\left[-\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}+\frac{m^2}{r^2}+k_l^2+\frac{2MV}{\hbar^2}\right]A_le^{ik_lz} = \frac{2ME}{\hbar^2}\sum_l A_le^{ik_lz}, \tag{A3}$$

where $k_l^2=(k-4\pi l/\lambda)^2$. The potential is multiplicatively separable into longitudinal and radial components, $V(z,r)=V^z(z)V^r(r)$.

To transform radial wavefunctions into Fourier space, we consider Eq(A1) and replace $\Psi(z,r)$ with $\Phi(z,r)=r^{1/2}\Psi(z,r)$. This leads to the Schrödinger equation:

$$-\frac{\partial^2\Phi}{\partial r^2}-\frac{\partial^2\Phi}{\partial z^2}+\left(\frac{m^2-\frac{1}{4}}{r^2}+\frac{2M(V-E)}{\hbar^2}\right)\Phi=0. \tag{A4}$$

We then produce the final version of the Schrödinger equation:

$$\sum_{l'}\sum_{n'}[\left(k_{l'}^2+\left(\tfrac{2\pi n'}{R}\right)^2\right)\delta_{l,l'}\delta_{j,j'} +\frac{\delta^{l,l'}}{R}\int_0^R\frac{m^2-\frac{1}{4}}{r^2}e^{i2\pi(n-n')r/R}dr + V^z_{l-l'}V^r_{n-n'}]\mathcal{A}_{l',n'} = \frac{2ME}{\hbar^2}\mathcal{A}_{l,n} \tag{A5}$$

where

$$V_l^z=\frac{2}{\lambda}\int_{\frac{\lambda}{4}}^{\frac{\lambda}{4}}V^z(z)\frac{2M}{\hbar^2}e^{4\pi ilz/\lambda}dz \tag{A6}$$

and

$$V_n^r=\frac{1}{R}\int_0^R V^r(r)e^{2\pi inr/R}dr \tag{A7}$$

and

$$\Phi_k(r,z)=\sum_{l=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}A_{l,n}e^{ik_lz}e^{-i2\pi nr/R}. \tag{A8}$$

This is now in a suitable form to perform a numerical calculation of the atomic energy spectrum.

This seems an unusual numerical method for solving the Schrodinger equation in cylindrical coordinates, as the most obvious transformation to make on Eq.(A3) is the Hankel transform, which expands the radial wavefunctions in terms of Bessel functions and removes the singularity. If we do this using the notation $\mathcal{A}_l^m(\kappa)=\int_0^\infty dr\, rA_l(r)J_m(\kappa r)$ we can show that:

$$\int_0^\infty d\kappa'\sum_{l'}\left\{(\kappa'^2+k_{l'}^2)\delta_{l,l'}\delta(\kappa-\kappa') +V^z_{l-l'}\kappa'V^r(\kappa,\kappa')\right\}\mathcal{A}_{l'}^m(\kappa')=\frac{2ME}{\hbar^2}\mathcal{A}_l^m(\kappa) \tag{A9}$$

where

$$V^r(\kappa,\kappa')=\int V^r(r)rJ_m(\kappa r)J_m(\kappa' r)dr \tag{A10}$$

and

$$V_l^z=\frac{2M}{\hbar^2}\frac{2}{\lambda}\int_{-\frac{\lambda}{4}}^{\frac{\lambda}{4}}V^z(z)e^{i4\pi lz/\lambda}dz \tag{A11}$$

For the purpose of producing a numerical calculation, the indices on the wavefunction components must be reduced to a finite set. Placing the Hankel coordinate κ on a grid is unsatisfactory, as there is very slow convergence for the integral defining $V^r(\kappa,\kappa')$, and it converges very slowly for large κ. This is why a better numerical performance can be achieved by transforming Eq.(A3) into Fourier space.

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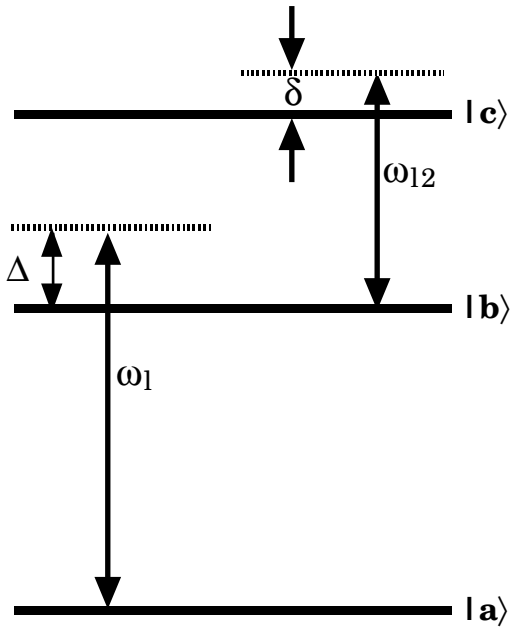
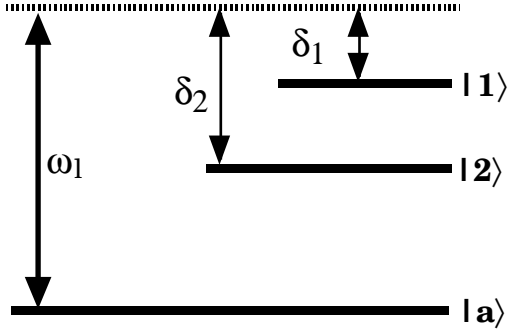
FIG. 1. Atomic states and laser configurations

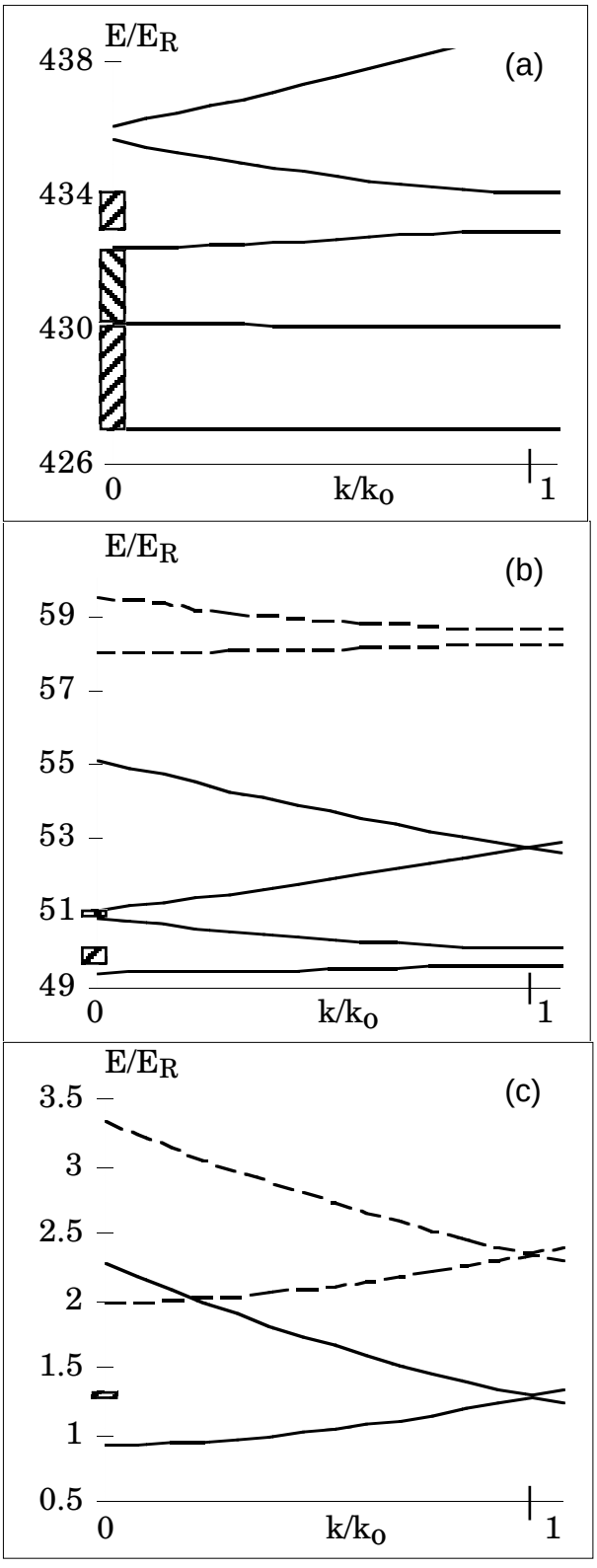
FIG. 2. Dressed states

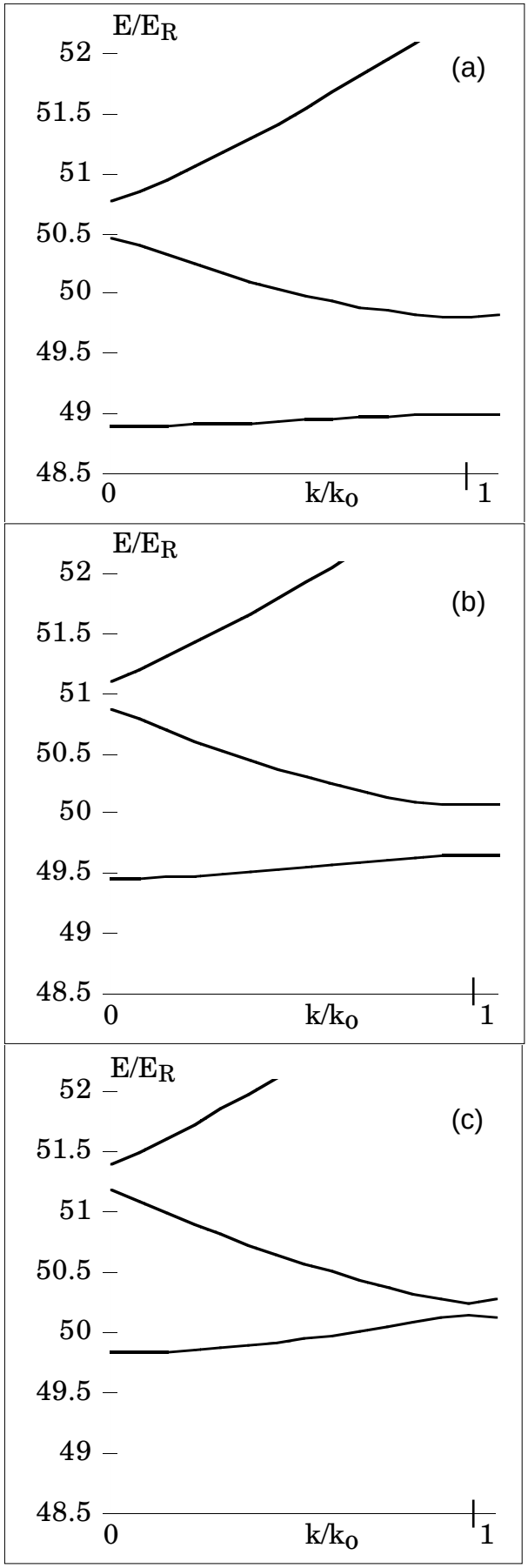
FIG. 3. The energy spectrum of atoms in a hollow fiber with increasing hole radius. The horizontal axis is quasimomentum $\hbar k$ in units of the momentum of a single photon $\hbar k_o$ from the confining laser. Energy is measured in units of the recoil energy $\mathrm{E}_R = (\hbar k)^2/(2M)$of a single atom. Note that the energy scale is different in each figure, as the atoms are immersed in a more intense light field when the fiber has a smaller hole. The dashed lines show the higher rotational mode, m=1, and the solid lines indicate the lowest rotational mode, m=0. Higher transverse modes in the m=0 spectrum are not shown in (b) and (c), for clarity. (a), (b) and (c) have hole radii of 0.25μm, 0.5μm, and 1.0μm respectively. These figures have a modulation of $M = 1 - (\min(V^z)/\max(V^z)) = 0.02$, as it was in Fig. 4(b).

FIG. 4. The energy spectrum for atoms in a hollow fiber with increasing modulation of the potential. The horizontal axis is quasimomentum $\hbar k$ in units of the momentum of a single photon $\hbar k_o$ from the confining laser. Energy is measured in units of the recoil energy $\mathrm{E}_R = (\hbar k)^2/(2M)$of a single atom. The modulation is measured by the parameter $M = 1 - (\min(V^z)/\max(V^z))$ where V^z is the z-dependence of the confining potential. (a), (b) and (c) have values for M of 0.04, 0.02 and 0.005 respectively. The hole radius for all three figures was 0.5μm, as it was in Fig. 3(b).


δ
|c⟩
ω12
Δ
|b⟩
ω1
|a⟩


δ1
δ2
ω1
|1⟩
|2⟩
|a⟩


E/E_R
438
434
430
426
(a)
0
k/k_o
1
E/E_R
59
57
55
53
51
49
(b)
0
k/k_o
1
E/E_R
3.5
3
2.5
2
1.5
1
0.5
(c)
0
k/k_o
1


E/E_R
52
51.5
51
50.5
50
49.5
49
48.5
0
k/k_o
1
(a)
E/E_R
52
51.5
51
50.5
50
49.5
49
48.5
0
k/k_o
1
(b)
E/E_R
52
51.5
51
50.5
50
49.5
49
48.5
0
k/k_o
1
(c)